Statistical and Low Temperature Physics.

32 lectures
- ~22 statistical
- ~10 low temp.

4 tutorials.

Essential book.

Statistical Physics.

Tony Guenault.

Q1. What is statistical mechanics?

Q2. What type of problems does it tackle?

Q3. What are its aims?

A2. Example – type of problem

Box of gas – many atoms in random motion.

Can be described in 2 ways.

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Macroscopic description.

Specify

Mass of gas — n mols.

Pressure P

Volume V

Gas law gives T via

$$PV = n\underbrace{R}_{\text{gas constant}}T$$

Described in terms of

laboratory measureable quantities

(4)

Microscopic description

N atoms equivalent to n mols

$x_1, y_1, z_1, p_{x_1}, p_{y_1}, p_{z_1}$ — components of instantaneous position and mtm for atom 1.

and the same for all N atoms.

Other answers to Q1, Q2, Q3

A1. Statistical mechanics – theory that connects microscopic and macroscopic descriptions.

A3 Start with microscopic picture – by summing and averaging predict laboratory measureables.

and their variation (usually with temperature T).

Points.

(i) Microscopic picture may be classical (kinetic theory) but usually quantum mechanical.

(ii) Other systems — conduction electrons, electron pairs (superconductors), phonons ...

(iii) Microscopic energy carriers (atoms in gas) need to be weakly interacting.

interacting — so can reach equilibrium

weakly — can associate energy ϵ with given atom.

⑥ Vocabulary

Macrostate.

Description of state in terms of laboratory measurables.

To begin – simple case

– choose macrostate to be isolated system

Means

(i) fixed number of particles N

(ii) fixed energy U

(iii) fixed volume V

Conditions

(ii) system does not exchange energy with surrounding's

(iii) no work $W = -\int P dV$ done on or by system.

Microstate.

Classical.

Position (x, y, z) and momentum (p_x, p_y, p_z) components for every atom..

$6N$ bits of instantaneous information

N typically $\sim 10^{23}$ (mol)

Quantum.

Microstate given by wavefunction

$\psi(1, 2 \, . \, . \, . \, . \, . \, . \, . \, N)$

Non (weakly) interacting system

W/f is $\psi(1) . \psi(2) \, . \, . \, . \, . \quad \psi(N)$.

atom 1.

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Wavef^{ns} must obey (ii)

$$\epsilon_1 + \epsilon_2 + \epsilon_3 \ldots \epsilon_N = U$$

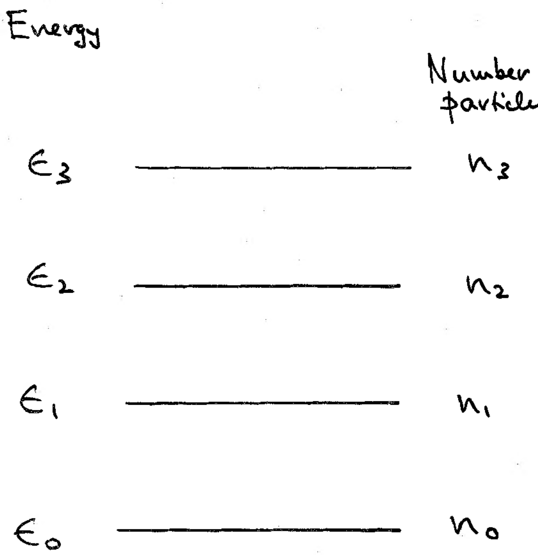
Number of different w/f with same total energy U = number of microstates Ω

Ω is very large number.

Basic Assumption

Each allowed microstate is equally likely.

Distributions – of weakly interacting particles in quantum states.



Must obey $\sum_j n_j = N$

$$\sum_j n_j \epsilon_j = U$$

Distribution $(n_0, n_1 \ldots\ n_j)$ written $\{n_j\}$

Many microstates in same $\{n_j\}$

Number microstates / distrib^n written $t(\{n_j\})$

Distribution in levels.

Same as above in states

except level has degeneracy g_i

for state at energy ϵ_i

Then
$$\sum_i g_i n_i = N$$

$$\sum_i g_i \epsilon_i n_i = U$$

Example – marks of class of students

Macrostate description } – average mark 51%.

Microstate description } – full class list of names and marks

Distribution description } Histogram of numbers of students in 10% bins of marks

General method to find distribution $\{n_j\}$

Step 1. Quantum mechanics to find energy states of single particles.

Step 2. Enumerate particle distributions

Step 3. Evaluate number of microstates for each distribution

Step 4. Calculate weighted distribution

Example with small number of distinguishable particles

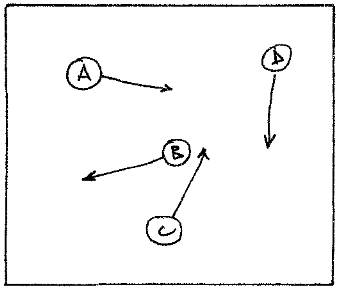
— see sheet.

Example 1.

Number of particles $N = 4$

Distinguishable A, B, C, D.

Total energy $U = 4\epsilon$



Step 1. Do quantum mechanics – find energy states.

Energy	Population
4ϵ	n_4
3ϵ	n_3
2ϵ	n_2
ϵ	n_1
0	n_0

Step 2 Particle distributions **Step 3.** Microstates / distribution

Distribution	n_0	n_1	n_2	n_3	n_4		
1	3	0	0	0	1	$t_1 = 4$	– Point 1
2	2	1	0	1	0	$t_2 = 12$	– Point 2
3	2	0	2	0	0	$t_3 = 6$	Point 3
4	1	2	1	0	0	$t_4 = 12$	Point 4
5	0	4	0	0	0	$t_5 = 1$	Point 5

Total number $= 35 = \Omega$.

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Point 1 A or B or C or D in 4ϵ state $t_1 = 4$

Point 2 4 choices for 3ϵ state, 3 for ϵ state $t_2 = 4 \times 3 = 12$

Point 3 Choose 2 from 4 in ${}^4C_2 = \frac{4!}{2!\,2!}$ ways $t_3 = \frac{4\times 3}{1\times 2} = 6$

Point 4 4 choices for 2ϵ state, 3 for 0 state $t_4 = 4\times 3 = 12$

Point 5. 1 way only $t_5 = 1.$

Step 4. Evaluate average populations of states

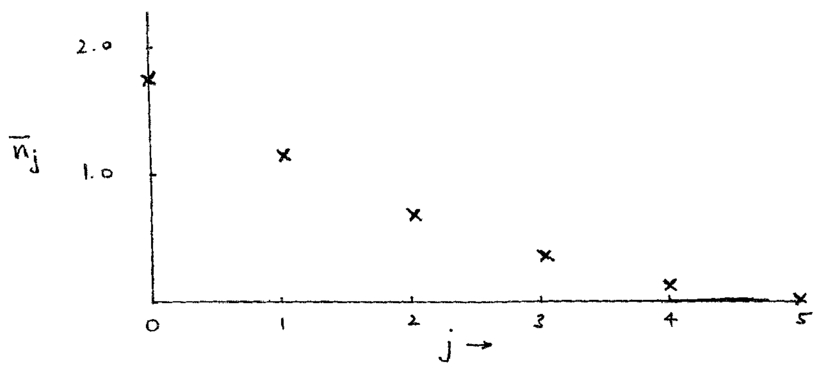
$\epsilon = 0$

$$\bar{n}_0 = \frac{4}{35}\times 3 + \frac{12}{35}\times 2 + \frac{6}{35}\times 2 + \frac{12}{35}\times 1 + \frac{1}{35}\times 0 = 1.71$$

Similarly $\bar{n}_1 = 1.14$ $\bar{n}_2 = 0.69$

$\bar{n}_3 = 0.34$ $\bar{n}_4 = 0.11$ $\bar{n}_5 = 0$

Plot $\bar{n}_j$ vs j

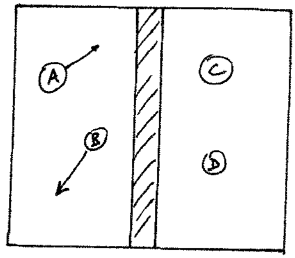


Example 2.

Divide previous system into enclosures 1 and 2

Enclosure 1 $\quad N_1 = 2 \quad$ A and B

Enclosure 2 $\quad N_2 = 2 \quad$ C and D



Energies $\quad U_1 = 4\epsilon$

$U_2 = 0 \qquad \Omega_2 = 1$

→ just 1 state C and D in $\epsilon = 0$.

Similar analyses for Enclosure 1.

Distribution	n_0	n_1	n_2	n_3	n_4	t
1	1	0	0	0	1	$t_1 = 2$
2	0	1	0	1	0	$t_2 = 2$
3	0	0	2	0	0	$t_3 = 1$
					Total Ω_1 =	5

Total number microstates $\Omega = \Omega_1 \times \Omega_2 = 5 \times 1 = 5$

Average state populations

Enclosure 1. $\qquad\qquad$ Enclosure 2

${}_1\bar{n}_0 = \frac{2}{5} \times 1 = 0.4 \qquad {}_2\bar{n}_0 = 2$

${}_1\bar{n}_1 = \frac{2}{5} \times 1 = 0.4 \qquad {}_2\bar{n}_1 = 0$

${}_1\bar{n}_2 = \frac{1}{5} \times 2 = 0.4 \qquad {}_2\bar{n}_2 = 0$

Division causes less microstates.

Relation between entropy S and number of microstates Ω

Propose $S = k \ln \Omega$

where k is Boltzmann constant.

Points

(i) Trial equation - judge it by correctness of its predictions

(ii) S is macroscopic quantity

Ω is microscopic quantity

This is bridge equation.

(iii) Reasonable form of relation

Total entropy of system of 2 parts 1 & 2 is $S = S_1 + S_2$

Total number of microstates $\Omega = \Omega_1 \times \Omega_2$

Implies

$$S = (\text{const}) \cdot \ln \Omega$$

(iv) This S same as that defined by

$$dS = \frac{đQ}{T}$$

(v) At low temperature if all particles go to ground state $\epsilon = 0$

$$\left.\begin{aligned} \Omega &= 1 \\ S &= 0 \end{aligned}\right\} \text{ 3rd Law of Thermodynamics.}$$

though must in practice consider frozen in disorder.

Statistical mechanics on system of distinguishable particles.

System.

Solid – large number of atoms $N \sim 10^{23}$.

– atoms weakly interacting

– distinguishable by Xtal site.

Aim. – deduce thermal equilibrium distribution – ie number of atoms in each energy state.

Step 1. Find energy states for single atom

$\epsilon_0, \epsilon_1, \epsilon_2 \ldots \epsilon_j$

Step 2. Form possible distributions of atoms in these states

$\{n_j\} \equiv$ set of populations $n_1, n_2 \ldots$ in levels $\epsilon_1 \ \epsilon_2 \ldots$

Conditions.

$$\sum_j n_j = N$$

$$\sum_j n_j \epsilon_j = U$$

Step 3. Count microstates corresponding to distribution $\{n_j\}$

Number microstates $t(\{n_j\}) = \dfrac{N!}{n_1! \, n_2! \ldots \, n_j!}$

$$= \frac{N!}{\prod_j n_j!}$$

- Justification - see sheet.

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Justification of $t(\{n_j\}) = \dfrac{N!}{n_1!\, n_2! \,\ldots\, n_j!}$

Problem equivalent to.

In how many ways can N objects be arranged if they are split up into j piles with n_1 in pile 1, n_2 in pile 2 ... n_j in pile j — the ordering in the piles being unimportant? This is $t(\{n_j\})$.

Line of N objects (distinguishable) can be arranged in N! ways.

If line of N objects now split into $n_1 + n_2 + \ldots n_j = N$

All different arrangements within pile 1 count as same distribⁿ. There are $n_1!$ of these.

Same for n_2, n_3 ... n_j

So number of distinct distribⁿˢ of N objects into $n_1, n_2 \ldots n_j$ piles

$$= t(\{n_j\}) = \frac{N!}{n_1!\; n_2! \;\ldots\; n_j!}$$

Many different distributions — corresponding to different ways of sharing N particles among j states — but some distributions much more probable (larger number of microstates) than others.

Surprise simplification.

For large $N \sim 10^{23}$

Most probable distribution $\{n_j^*\}$ has so many more microstates than any other distribution that we can ignore all other distributions.

Justification — see sheet.

Means $t(\{n_j^*\}) \equiv t^* = \Omega$